

St. Aloysius (Autonomous) College, Jabalpur
Department of Chemistry

M.Sc. (CHEMISTRY)
(FOUR SEMESTER COURSE)

Choice Based Credit system is implemented in PG Chemistry since 2018-19. Each semester has core and elective papers with 4 credits and 2 practical papers of 2 credits each.

Distribution of Credits in Each Semester

M.Sc I + II Semester

4 Core paper – 04 Credits each	$4 * 4 = 16$ Credits
1 Elective paper – 04 Credits	$1 * 4 = 4$ Credits
2 Practical's – 02 Credits each	$2 * 2 = 4$ Credits
Skill Development – 01 Credit	$1 * 1 = 1$ Credits
Tutorial – 01 Credit	$1 * 1 = 1$ Credits
Total Credits	26 Credits

M.Sc III Semester

3 Core paper – 04 Credits each	$3 * 4 = 12$ Credits
2 Elective paper – 04 Credits	$2 * 4 = 8$ Credits
2 Practical's – 02 Credits each	$2 * 2 = 4$ Credits
Skill Development – 01 Credit	$1 * 1 = 1$ Credits
Tutorial – 01 Credit	$1 * 1 = 1$ Credits
Total Credits	26 Credits

M.Sc IV Semester

2 Core paper – 04 Credits each	$2 * 4 = 8$ Credits
2 Elective – 04Credits	$2 * 4 = 8$ Credits
1 Minor Project/Dissertation/Internship	5 Credits
Skill Development – 01 Credit	$1 * 1 = 1$ Credits
Total Credits	22 Credits
Grand Total of Credits	100 Credits

SEMESTER I

Course No.	Course	Credit	Theory Marks	CIA Marks
Course MCH 101	Inorganic Chemistry	4	50	50
Course MCH 102	Organic Chemistry	4	50	50
Course MCH 103	Physical Chemistry	4	50	50
Course MCH 104	Spectroscopy	4	50	50
Course MCH 105	Biology/Maths for Chemist and Computers	4	50	50
Course MCH 106	Inorganic Chemistry Practical	2	50	50
Course MCH 107	Physical Chemistry Practical	2	50	50
Total			350	350
Grand Total			700	

SEMESTER II

Course No.	Course	Credit	Theory Marks	CIA Marks
Course MCH 201	Inorganic Chemistry	4	50	50
Course MCH 202	Organic Chemistry	4	50	50
Course MCH 203	Physical Chemistry	4	50	50
Course MCH 204	Spectroscopy I	4	50	50
Course MCH 205 Elective	MCH 205 A Analytical Chemistry MCH 205 B Photochemistry (Any One from MCH 205A-B)	4	50	50
Course MCH 206	Organic Chemistry Practical	2	50	50
Course MCH 207	Inorganic Chemistry Practical	2	50	50
Total			350	350
Grand Total			700	

SEMESTER III

Course No.	Course	Credit	Theory Marks	CIA Marks
Course MCH 301	Inorganic Chemistry	4	50	50
Course MCH 302	Physical Chemistry	4	50	50
Course MCH 303	Spectroscopy II	4	50	50
Course MCH 304 I Elective	Course MCH 304 A Medicinal Chemistry Course MCH 304 B Chemistry of Natural Products Course MCH 304 C Polymer (Any Two from MCH304 A to C)	4	50	50
Course MCH 304 II Elective		4	50	50
Course MCH 305	Organic Chemistry Practical	2	50	50
Course MCH 306	Physical Chemistry Practical	2	50	50
Total			350	350
Grand total			700	

SEMESTER IV

Course No.	Course	Credit	Theory Marks	CIA Marks
Course MCH 401	Inorganic Chemistry	4	50	50
Course MCH 402	Organic synthesis strategies	4	50	50
Course MCH 403 Departmental Elective	Course MCH 403 A Environmental Chemistry Course MCH 403 B Chemistry of materials (Any One from MCH403A or 403 B)	4	50	50
Course MCH 404 Open Elective	Course MCH 404 A Biochemistry Course MCH 404B Bioorganic Chemistry	4	50	50
Course MCH 405	Minor Project/Dissertation/Internship	5	100	
Total			300	200
Grand Total			500	

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. I SEM	Core	Course MCH 101	Inorganic Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE

To develop an understanding of structure and chemical bonding present in inorganic compounds and the basic concept of *Reaction Mechanism of Transition Metal Complexes*.

UNIT I

Stereochemistry and Bonding in Main Group Compounds. VSEPR theory and its application for treating structures of inorganic molecules and ions containing lone pairs of electrons, shortcomings of VSEPR model. MO treatment of polyatomic molecules, e.g., ozone, nitrite, nitrate, hydrazoic acid and benzene.

UNIT II

Metal-Ligand Bonding. Molecular orbital theory. Qualitative aspects of metal-ligand sigma-bonding in octahedral, tetrahedral and square planar complexes. Jahn-Teller Effect *Electronic Spectra and of Transition Metal Complexes*. Spectroscopic term, terms and microstates for the p^2 and d^2 configurations, Hund's rules for ground state terms, the correlation of spectroscopic terms into Mulliken symbols, electronic transition selection rules, Orgel diagrams for transition metal complexes (d^1 - d^9 states). Jahn-teller effect and electronic spectra of complexes

UNIT III

Metal-Ligand Equilibria in Solution. Stepwise and overall formation constants and their relationship, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by Bjerrum method, Job's and Mole ratio methods.

UNIT IV

Reaction Mechanism of Transition Metal Complexes I. Inert and labile complexes, interpretation of lability and inertness of transition metal complexes on the basis of valence bond and crystal field theories. Kinetics of octahedral substitution: acid hydrolysis, factors affecting acid hydrolysis.

UNIT V

Reaction Mechanism of Transition Metal Complexes II. Base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism. Substitution reactions in square planar complexes: The *Trans* effect and the *trans* influence: Polarization and Pi-Bonding theories, applications of *Trans* effect in synthesis, Kurnakove's test of distinguishing *cis* and *trans* isomers using the concept of trans effect, mechanism of substitution reactions in square planar complexes, factors affecting substitution reactions. Acquaintance of *Trans* effect in octahedral complexes.

Course outcome:

By the end of this course student will be able to-

- Gain a thorough knowledge about VSEPR theory and its applications for treating the structure of simple inorganic and polyatomic molecules and ions.
- Build the concept of Metal Ligand Bonding and equilibria in solution state.
- Develop an understanding about electronic spectra of transition metal complexes.
- Develop the concept of reaction mechanism in transition metal complexes and factors affecting the reactions in square planar and octahedral complexes.

Suggested Reading

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row.
3. Chemistry of the Elements. N.N. Greenwood and A. Earnshaw, Pergamon.
4. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
5. Magnetochemistry, R.I. Carlin, Springer Verlag.
6. Comprehensive Coordination Chemistry eds., G. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon

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M.Sc. I SEM	Core	Course MCH 102	Organic Chemistry	Max: 40	Min: 14

Course Objective:

To develop an understanding of reactivity, structure and bonding, mechanisms, stereochemistry and aliphatic and aromatic substitution reactions of organic compounds

UNIT I

Structure and Bonding. Bonding in organic molecules. Delocalized chemical bonding-conjugation, cross conjugation, Conjugation, resonance, hyperconjugation. Aromaticity in benzenoid and non-benzenoid compounds, alternate and non-alternate hydrocarbons. Hückel rule, anti-aromaticity, homo-aromaticity. Bonds weaker than covalent bond. Hydrogen bonding, crown ether complexes, and cyclodextrins

UNIT II

Stereochemistry. Chirality, elements of symmetry, molecules with more than one chiral center, threo and erythroisomers. R and S configuration. Separation of enantiomers. Regioselective, stereospecific and stereoselective reactions. Asymmetric synthesis. Optical activity in the absence of chiral carbon (atropisomerism) biphenyls, allenes and spiranes, and their nomenclature. Conformational analysis of cyclohexanes and decalins. Effect of conformation on reactivity

UNIT III

Reaction Mechanism. Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, and control, Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. Effect of structure on reactivity -resonance and field effects, steric effect. The Hammett equation and linear free energy relationship, substituent and reaction constants. Taft equation.

UNIT IV

Aliphatic Nucleophilic Substitution. The S_N2 , S_N1 , mixed S_N2 and S_N1 , and SET mechanisms. The S_Ni mechanism. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium. The neighbouring group mechanism, neighbouring group participation by Pi and Sigma bonds. Classical and nonclassical carbocations, norbornyl system, carbocation rearrangements

UNIT V

Aromatic Nucleophilic Substitution. The S_NAr , S_N1 , benzyne and $S_{RN}1$ mechanisms. Reactivity, effect of substrate structure, leaving group and attacking nucleophile. Bucherer reaction, alkylation, and amination. The Bamberger rearrangement. The von Richter rearrangement

COURSE OUTCOME:

By the end of this course student will be able to-

- Develop concepts of the fundamentals, structure and bonding, stereochemistry and reaction mechanism in organic compounds.
- Enhance the knowledge about Aliphatic and Aromatic Nucleophilic Substitution reactions with suitable examples of some known organic chemical reactions.
- Understand the fundamentals in organic chemistry about Aromaticity, Molecular chirality, thermodynamic and kinetic control of reactions and its applications

SUGGESTED READING

1. Organic Chemistry, J. Claden, N. Greeves, S. Warren, P. Wothers, Oxford University Press.
2. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, Wiley-Interscience.
3. Organic Chemistry, P.Y. Bruice, Pearson Education Asia.
4. Organic Chemistry, L.G. Wade, Jr., Pearson Education.
5. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
6. Organic Chemistry, J. McMurry, Thomson Asia.
7. Organic Chemistry, T.W.G. Solomons and C.B. Fryhle, John Wiley (Asia).
8. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman.
9. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice-Hall.
10. Stereochemistry of Organic Compounds, E.L. Eliel and S.H. Wilen, John Wiley (Asia).
11. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
12. Stereochemistry of Organic Compounds, P .S. Kalsi, New Age International.
13. Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman and G.S. Kriz, Thomson, Brooks/Cole.
14. Organic Spectroscopy, W. Kemp, ELBS, Macmillan.
15. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley
16. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
17. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tata McGraw-Hill.

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M.Sc. I SEM	Core	Course MCH 103	Physical Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE:

- To study the fundamentals and applications of classical and quantum mechanics
- To impart the knowledge of Chemical Dynamics to chain and enzyme catalysed reactions
- To learn the importance and utility of Chemical Thermodynamics and their role in chemistry.

UNIT I

Introduction to exact quantum mechanical results. The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to systems such as particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

UNIT II

Approximate Methods. The variation theorem, linear variation principle. Perturbation theory (introductory idea). Application of variation method to the Helium atom.

Angular Momentum. Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigen values of angular momentum, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

UNIT III

Classical Thermodynamics. Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies. Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significance. Determinations of these quantities. Concept of fugacity and determination of fugacity.

Derivation of phase rule and its application to three component systems, second order phase transitions.

UNIT IV

Chemical Dynamics (Part I). Methods of determining rate laws, Arrhenius equation, collision theory of reaction rates, steric factor, activated complex theory, ionic reactions, kinetic and thermodynamic control of reactions.

UNIT V

Chemical Dynamics (Part II). Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions, homogeneous catalysis, kinetics of enzyme reactions

COURSE OUTCOMES:

By the end of this course student will be able to-

- Understand quantum mechanical and classical thermodynamics principles.
- Develop an understanding of the Schrodinger equation and its applications, Perturbation theory and concept of Angular Momentum.
- Procure an in-depth knowledge about free energy, entropy and fugacity.
- Understand and apply the concepts of chemical dynamics to organic reactions and dynamic chain reactions

SUGGESTED READINGS

1. Prasad, R. K. (2014). Quantum Chemistry (IV Revised Edition). New Delhi: New Age International Publishers Pvt. Ltd.
2. Chandra, A. K. (2017). Quantum Chemistry (IV Edition). New Delhi: Tata McGraw – Hill Publishing Company Ltd.
3. House, J. E. (2004). Fundamental of Quantum Chemistry (II Edition). New Delhi: Academic Press.
4. Levine, I. N. (2016). Quantum Chemistry (VII Edition). New Delhi: Pearson Education Pvt. Ltd.
5. Puri, B. R., Sharma, L. R., & Pathania, M. S. (2013). Principles of Physical Chemistry (46th Edition). Jalandar: Vishal Publishing Co.
6. Atkins, P., & De Paula, J. (2014). Atkins Physical Chemistry (X Edition). Oxford: Oxford University Press.

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M.Sc. I SEM	Core	Course MCH 104	Spectroscopy I	Max: 40	Min: 14

COURSE OBJECTIVE

To understand the principle, theories, instrumentation and applications of Microwave, FT-IR, Raman and Microwave spectroscopic techniques

UNIT I

Unifying Principles. Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, transition moment, selection rules, intensity of spectral lines.

UNIT II

Microwave Spectroscopy. Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field. Applications.

UNIT III

Infrared Spectroscopy. Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P,Q,R branches. Vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region.

UNIT IV

Raman Spectroscopy. Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

UNIT V

Electronic Spectroscopy. Atomic Spectroscopy. Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms. Molecular Spectroscopy. Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, charge-transfer spectra.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand the concept Microwave, Infrared, Raman and Electronic spectroscopy and its applications.
- Develop an understanding of Atomic and Molecular spectroscopy.

SUGGESTED READING

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Applied Electron Spectroscopy for chemical analysis d. H. Windawi and F.L. Ho, Wiley Interscience.
3. NMR, NQR, EPr and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Harwood.
4. Physical Methods in Chemistry, R.S. Drago, Saunders College.
5. Chemical Applications of Group Theory, F.A. Cotton.
6. Introduction to Molecular Spectroscopy, G.M. Barrow, Mc Graw Hill.
7. Basic Principles of Spectroscopy, R. Chang, Mc Graw Hill.
8. Theory and Application of UV Spectroscopy, H.H. Jaffe and M. Orchin, IBH Oxford.
9. Introduction to Photoelectron Spectroscopy, P.K. Ghosh, John Wiley.
10. Introduction to Magnetic Resonance. A Carrington and A.D. Maclachalan, Harper & Row.

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M.Sc. I SEM	Elective	Course MCH 105	Maths for Chemist and Computers (Theory)	Max: 40	Min: 14

COURSE OBJECTIVE:

- This course introduces the math content to chemistry students. It has been designed to complement lecture material with particular focus on the application of maths in chemistry.
- To enable students to learn and implement the basics of computer in chemical sciences.

UNIT - I

Vectors. Vectors, dot, cross and triple products etc. gradient, divergence and curl, Vector Calculus.

Matrix Algebra. Addition and multiplication; inverse, adjoint and transpose of matrices.

UNIT- II

Differential Calculus. Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.).

Integral calculus. Basic rules for integration, integration by parts, partial fractions and substitution. Reduction formulae, applications of integral calculus. Functions of several variables, partial differentiation, co-ordinate transformations (e.g. Cartesian to spherical polar).

UNIT - III

Elementary Differential equations. First-order and first degree differential equations, homogenous, exact and linear equations. Applications to chemical kinetics, secular equilibria, quantum chemistry etc. second order differential equation and their solutions.

Permutation and Probability. Permutations and combinations, probability and probability theorems average, variance root means square deviation examples from the kinetic theory of gases etc., fitting (including least squares fit etc with a general polynomial fit).

UNIT-IV:

Basic structure of a computer: The CPU, the I/O devices, the internal memory, commonly used secondary storage media. Data representation: The software: Concept of low level and high level languages, Compiler interpreter, editor, operating system concepts, Windows operating systems, salient features of MS-office with special emphasis on MS Excel (graphs, tables, formulas)

UNIT-V:

Programme Development Process Algorithm, Flowchart, Decision-table, elements of high level programming languages. Input-output statements, conditional statements, control structure,

concept of data file, file operations like searching, storing, with reference to C/ C++ Programming.

COURSE OUTCOME

By the end of this course student will be able to-

- Understand fundamental concepts of Maths in the field of Chemistry and allied subjects.
- Build concepts in fundamental Maths which would bridge the gap between Chemistry and Physical sciences.
- Enhance understanding and applicability of concepts in varied fields of Physical, Chemical and Biological Sciences

SUGGESTED READING

1. The chemistry Mathematics Book, E.Steiner, Oxford University Press.
2. Mathematics for chemistry, Doggett and Suiclific, Logman.
3. Mathematical for Physical chemistry : F. Daniels, Mc. Graw Hill.
4. Chemical Mathematics D.M. Hirst, Longman.
5. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall.
6. Basic Mathematics for Chemists, Tebbutt, Wiley.
7. Mathematics for Chemists: Bhupendra Singh, Pragati Prakashan
8. Fundamentals of Computer : V. Rajaraman, Prentice Hall.
9. Computers in Chemistry : K.V. Raman, Tata Mc Graw Hill).
10. Computer Programming in FORTRAN IV-V Rajaraman, Prentice Hall.
11. Computers and Common Sense, R. Hunt and J. Shelley, Prentice Hall.
12. Computational Chemistry, A.C. Norris.
13. Microcomputer Quantum Mechanics, J.P. Killngbeck, Adam Hilger.
14. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, Prentice Hall.

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M.Sc. I SEM	Elective	Course MCH 105	Biology for Chemist and Computers	Max: 40	Min: 14

COURSE OBJECTIVE:

- This course introduces the Biology content to chemistry students
- To study the structure and organization of cell membrane and cell wall, process of membrane transport and membrane models.
- To enhance understanding and applicability of concepts in varied fields of Physical, Chemical and Biological Sciences.
- To enable students to learn and implement the basics of computer in chemical sciences.

UNIT - I

Cell Structure and Functions. Structure prokaryotic and eukaryotic cells, intracellular organelles and their functions, comparison of plant and animal cells. Overview and their functions, comparison of plant and animal cells. Overview of metabolic processes-catabolism and anabolism. ATP – the biological energy currency. Origin of life-unique properties of carbon chemical evolution and rise of living systems. Introduction to bio-molecules, building blocks of biomacromolecules.

UNIT - II

Carbohydrates. Conformation of monosaccharides, structure and functions of important derivatives of mono-saccharides like glycosides, deoxy sugars, myoinositol, amino sugars. Nacetylmuramic acid, sialic acid disaccharides and polysaccharides. Structural polysaccharides cellulose and chitin. Storage polysaccharides-starch and glycogen. Structure and biological function of glucosaminoglycans of mucopolysaccharides. Carbohydrates of glycoproteins and glycolipids. Role of sugars in biological recognition. Blood group substances. Ascorbic acid.

UNIT - III

Amino-acids, Peptides and Proteins. Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins. Force responsible for holding of secondary structures. α helix, β sheets, super secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure. Quaternary structure. Amino acid metabolism-degradation and biosynthesis of amino acids, sequence determination, chemical/enzymatic/mass spectral, racemization/detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

UNIT-IV:

Basic structure of a computer: The CPU, the I/O devices, the internal memory, commonly used secondary storage media. Data representation: The software: Concept of low level and high level languages, Compiler interpreter, editor, operating system concepts, Windows operating systems, salient features of MS-office with special emphasis on MS Excel (graphs, tables, formulas)

UNIT-V:

Programme Development Process Algorithm, Flowchart, Decision-table, elements of high level programming languages. Input-output statements, conditional statements, control structure, concept of data file, file operations like searching, storing, with reference to C Programming.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand fundamental concepts Biology in the field of chemistry and allied subjects.
- Build concepts in fundamental Biology which would bridge the gap between Chemistry and Physical /Biological sciences.
- Enhance understanding and applicability of concepts in varied fields of Physical, Chemical and Biological Sciences.

SUGGESTED READINGS:

1. Principles of Biochemistry, A.L. Lehninger, Worth Publishers.
2. Biochemistry, L. Stryer, W.H. Freeman.
3. Biochemistry, J. David Rawan, Neil Patterson.
4. Biochemistry, Voet and Voet, John Wiley.
5. Outlines of Biochemistry E.E. Conn and P.K. Stumpf, John Wiley.
6. Fundamentals of Computer : V. Rajaraman, Prentice Hall.
7. Computers in Chemistry : K.V. Raman, Tata Mc Graw Hill).
8. Computer Programming in FORTRAN IV-V Rajaraman, Prentice Hall.
9. Computers and Common Sense, R. Hunt and J. Shelley, Prentice Hall.
10. Computational Chemistry, A.C. Norris.
11. Microcomputer Quantum Mechanics, J.P. Killngbeck, Adam Hilger.
12. An Introduction to Digital Computer Design, V. Rajaraman and T. Radhakrishnan, Prentice Hall.

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M.Sc. II SEM	Core	MCH 201	Inorganic Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE

- To acquaint students with concept of symmetry and symmetry operations in chemistry.
- To develop advanced principles of bonding in inorganic compounds and their application.
- To develop an understanding of structure, bonding, properties and applications of boranes, borazines, carboranes, metallo carboranes and Metal nitrosyls

UNIT I

Reaction Mechanism of Transition Metal Complexes III.: Substitution reaction without Metal – Ligand bond cleavage. Oxidation reduction reactions through group transfer, through electron transfer, Inner sphere and outer sphere mechanism, 2 electron transfer reactions, Distinguish between Inner sphere and Outer sphere, factors affecting electron transfer reaction, Marcus – Hush theory

UNIT II

Metal Pi-Complexes. Metal carbonyls: structure and bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation. Dioxygen complexes, Wilkinson's catalyst

UNIT III

Borane Chemistry Metal Clusters. Bonding and topology of boranes, 4-digit coding (s, t, y, x) numbers for B₂H₆, B₄H₁₀, B₅H₉, B₅H₁₁ and B₆H₁₀ and their utilities. Acquaintance with carboranes and metallocarboranes. Metal clusters: synthesis, reactivity and bonding.

UNIT IV

Electronic Spectra and Magnetic Properties of Transition Metal Complexes. Calculations of Dq, B and β parameters for Cr(III), Co(II) and Ni(II) complexes using electronic spectral data. Charge transfer spectra: ligand to metal and metal to ligand.

UNIT V

Metal Pi-Complexes. Metal nitrosyls: Nitrosylating agents for synthesis of metal nitrosyls, vibrational spectra and x-ray diffraction studies of metal nitrosyls for bonding and structure elucidation, important reactions of transition metal nitrosyl complexes pertaining to potentiality in air pollution control, biomedical applications. Dinitrogen complexes, Vaska's compound

COURSE OUTCOME

By the end of this course student will be able to-

- Gain a thorough knowledge about Metal carbonyls and nitrosyls and their applications.
- Develop the concept of reaction mechanism in transition metal complexes and factors affecting the reactions in substitution reactions and electron transfer reactions
- Build the concept of Borane chemistry and metal clusters and their applications.

SUGGESTED READING

1. Raman, K.V. (2002). Group Theory and its Applications to Chemistry. New Delhi: Tata McGraw Publishing Company.
2. Cotton, F. A. (2003). Chemical Applications of Group Theory (III Edition). Texas: A Wiley Inter Science Publication.
3. Veera Reddy, K. (2009). Symmetry and Spectroscopy of Molecules. New Delhi: New Age International Pvt. Ltd.
4. Huheey, J. E., Keitler, E. A., & Keitler, R. L. (2012). Inorganic Chemistry Principles of Structure and Reactivity (IV Edition). Singapore: Pearson Education.
5. Malik. Wahid. U, Tuli. G. D and Madan, R.D. (2009). Selected Topics in Inorganic Chemistry New Delhi: S. Chand and Co.
6. Sarn, K. (2005). Co-ordination Chemistry.(Ist Edition) New Delhi: Rajat Publications.
7. Catherine, E. H., & Alan G. S. (2012). Inorganic Chemistry (IV Edition). England: Pearson Education Limited, Harlow.
8. Cotton, F. A., Wilkinson, G., & Paul. L. (2007). Basic Inorganic Chemistry (III Edition). New York: John Wiley & Sons. 6. Chakraborty, D. K. (2012). Inorganic Chemistry. (II Revised Edition) New Delhi: New Age International Publishing Pvt. Ltd.

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M.Sc. II SEM	Core	Course MCH 202	Organic Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE:

- To understand mechanistic and stereochemical aspects of addition reactions, versatile knowledge of different some named reactions and their application in organic synthesis.
- To learn about some familiar addition and elimination reactions and their reaction mechanisms
- To gain knowledge about pericyclic reactions, their mechanism and symmetry properties

UNIT I

Free Radicals. Free radical reactions and their stereochemistry. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, hydroperoxide formation, replacement of diazonium group. Hunsdiecker reaction.

UNIT II

Addition to Carbon-Carbon Multiple Bonds. Mechanistic and stereochemical aspects of addition reactions. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation. *Addition to Carbon-Hetero atom Multiple Bonds.* Mechanism of metal hydride reduction of carbonyl compounds, acids, esters and nitriles. Wittig reaction. Mechanism of condensation reactions involving enolates. Mannich, Benzoin, Perkin, and Stobbe reactions.

UNIT III

Elimination Reactions. The E2, E1 and E1cB mechanisms and their spectrum. Orientation of the double bond. Reactivity, effect of substrate structure, attacking base, the leaving group and the medium. Elimination *versus* substitution. Mechanism and orientation in pyrolytic elimination. The Hofmann degradation. Dihalo-elimination. Decomposition of toluene-p-sulphonyl hydrazones. Conversion of ketoximes to nitriles. *N*-Nitrosoamine to diazoalkane transformation

UNIT IV

Pericyclic Reactions: Part I. Molecular orbitals and their symmetry. Molecular orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system, and their symmetry properties.

Pericyclic reactions. Characteristics and classification. Electrocyclic reactions: conrotatory and disrotatory motions, $4n$, $4n+2$ and allyl systems. Woodward-Hoffmann correlation diagrams. FMO and PMO approach.

UNIT V

Pericyclic Reactions: Part II. Cycloadditions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Antarafacial and suprafacial additions. $4n$ and $4n+2$ systems, $2+2$ addition of ketenes. Ene synthesis.

Sigmatropic Rearrangements. Suprafacial and antarafacial 1,3- and 1,5- shifts of H, sigmatropic shifts involving carbon moieties, 2,3-, and 3,3-sigmatropic rearrangements. Claisen, Cope, aza-Cope, Sommet-Hauser, and Fisher Indole rearrangements.

Course Outcome:

By the end of this course student will be able to-

- Understand concepts of the pericyclic reactions and their symmetry properties.
- Enhance the knowledge about Elimination reactions, mechanism and some known examples.
- Procure an in-depth knowledge about free radical reactions and the mechanism of some known reactions.
- Build concepts of addition reactions to carbon –carbon and carbon –hetero atom multiple bonds and some famous named reactions.

SUGGESTED READINGS

1. Smith, M. B. (2015). March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure (VII Edition). New Jersey: John Wiley & Sons, Inc., Hoboken.
2. Peter Sykes, (1995). A guidebook to mechanism in Organic Chemistry (VI Edition). New York: John Wiley & sons Inc.
3. Sanyal, S. N. (2014). Reactions, Rearrangements and Reagents (IV Edition). New Delhi: Bharathi Bhawan (Publishers and Distributors).
4. Tewari, N. (2011). Advanced Organic Reaction Mechanism (III Edition). Kolkata: Books and Allied (P) Ltd.
5. Clayden, J., Greeves, N. & Warren, S. (2012). Organic Chemistry (II Edition). Oxford University Press, Oxford

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. II SEM	Core	Course MCH 203	Physical Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE:

To understand the general features of chemical dynamics, advanced concept of Adsorption, in-depth knowledge of Applied electrochemistry, corrosion and its applications.

UNIT I

Chemical Dynamics(Part III). General features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions and of barrierless chemical reactions in solution, probing the transition state. Dynamics of unimolecular reactions; Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus and Slater theories of unimolecular reactions.

UNIT II

Adsorption. Surface tension, capillary action, pressure difference across curved surface, Laplace equation, vapour pressure of droplets, Kelvin equation; Gibbs adsorption isotherm. Multilayer adsorption, BET equation. Calculation of surface area, catalytic activity at surfaces. Surface films on liquids; electrokinetic phenomena; surface active agents. Micellisation, hydrophobic interaction. Critical micellar concentration. Solubilisation. Donnan's membrane equilibria.

UNIT III

Electrochemistry of solutions. Debye-Huckel -Onsager treatment and its extension to concentrated solutions. Ion size factor and ion-solvent interactions. Concept of activity. Determination of mean ionic activity and activity coefficient. *Lippmann electrocapillary phenomenon.* Electrocapillary curves of mercury and their interpretation. Structure of electrified interfaces. Helmholtz, Guoy and Chapman and Stern models. Introductory idea of advancements in electrified surfaces. Electrokinetic potential, its determination and significance.

UNIT IV

Irreversible electrode phenomenon. Decomposition voltage and overvoltage. Consecutive electrode processes. Exchange current density. Butler-Volmer's equation. Tafel's plot. Theory of polarography. Ilkovic equation. Half wave potential and its significance. Introduction to corrosion. Forms of corrosion. Corrosion monitoring and prevention

UNIT V

Applied Electrochemistry Electrochemistry: Nernst equation, electrode kinetics, electrical double layer, Debye-Huckel theory. Voltammetry, Current voltage relationship, Characteristic of DME, Half wave potential. Amperometric titrations.

Course Outcome:

By the end of this course student will be able to-

- Understand Applied electrochemistry, corrosion and its applications
- Develop an understanding of the electrochemistry of solutions, irreversible electrode phenomenon and its applications,
- Procure an in-depth knowledge about adsorption phenomenon, its theories and applications.
- Understand and apply the concepts of chemical dynamics to fast reactions, unimolecular reactions and molecular motions.

SUGGESTED READINGS:

1. Glasstone, S. (2008). Thermodynamics for Chemists. New York: Litton Edition Publishing.
2. Atkins, P., & De Paula, J. (2014). Atkins Physical Chemistry (X Edition). Oxford: Oxford University Press.
3. Kapoor, K. L. (2015). Text Book Physical Chemistry Vol. V. New Delhi: MacMillan India Ltd.
4. Lavin, I. N. (2002). Physical Chemistry (V Edition). New Delhi: Tata-McGraw Hill Publishing Company.
5. Whittakar, A. G. (2001). Physical Chemistry. New Delhi: Mount & Heal Viva Books Pvt. Ltd.

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. II SEM	Core	Course MCH 204	Spectroscopy –II	Max: 40	Min: 14

COURSE OBJECTIVE:

To understand the theories of NMR, FT-IR, Photoelectron Spectroscopy, ESR spectroscopic techniques, their principle, instrumentation and applications.

UNIT –I

Infrared and Raman Spectroscopy. Instrumentation and sample handling. Calculation of vibrational frequencies. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, carbonyl compounds, alcohols, ethers, amines, phenols and aromatic compounds. Finger-print region. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FT-IR. Resonance Raman effect. Concept and factors that influence group frequencies.

UNIT- II

Electronic Spectroscopy and its applications. Electromagnetic radiation, wavelength, wave number, frequency, and energy calculation. Electronic transitions (185-800 nm), Beer-Lambert law, effect of solvent on electronic transitions, Fieser-Woodward rules for conjugated dienes and carbonyl compounds. *Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD).* Concept of ORD and CD, deduction of absolute configuration, octant rule for ketones.

UNIT -III

Nuclear Magnetic Resonance Spectroscopy. ^1H -NMR phenomenon. Chemical shift, shielding and deshielding mechanism, mechanism of measurement, chemical shift values and its correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercapto). Chemical exchange, effect of deuteration. Spin-spin coupling (first order spectra; AX, AB, AMX spectra). Coupling constant, Karplus curve. Complex spin-spin interactions. Simplification of complex spectra, nuclear magnetic double resonance, increased field strength, contact shift reagents. Nuclear Overhauser effect (NOE). FT technique.

Nuclear Magnetic Resonance Spectroscopy. *NMR Shift reagents, shift mechanism and its utility in simplification of NMR spectra. Applications of NMR in characterization of coordination compounds*

UNIT -IV

Electron Spin Resonance Spectroscopy. Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the g value. Hyperfine coupling. Double resonance in esr. Spin Hamiltonian relationship, measurement techniques, applications.

UNIT- V

Photoelectron Spectroscopy. Basic principles; photo-electric effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Auger electron spectroscopy -basic idea.

Photoacoustic Spectroscopy. Basic principles of photoacoustic spectroscopy (PAS), chemical and surface applications

Course Outcome:

By the end of this course student will be able to-

- Understand organic spectroscopy, its types and applications in structure elucidation and identification.
- Develop an understanding of Infrared, Raman and Electronic spectroscopy and its applications.
- Develop an understanding of Nuclear Magnetic Resonance and its applications.
- Build the concept of Photoelectron spectroscopy and photoacoustic spectroscopy and its applications in structure elucidation.

SUGGESTED READING

1. Modern Spectroscopy, J.M. Hollas, John Wiley.
2. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.
3. Physical Methods in Chemistry, R.S. Drago, Saunders College.
4. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
5. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
6. Introduction to Photoelectron Spectroscopy: P. K. Ghosh, John Wiley.
7. Macromolecules: Structure and Function, F. Wold, Prentice Hall.
8. Fundamentals of molecular spectroscopy, C.N. Banwell, Tata McGraw-Hill, New Delhi.
9. Instrumental Methods of Analysis, Willard, Meritt and Dean.

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. II SEM	Elective (A)	Course MCH 205	Analytical Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE:

To provide the students an in-depth account of various modern analytical techniques like spectrophotometry, XRD, AAS, thermal and electroanalytical techniques and Chromatography, their principles, instrumentation and applications

UNIT I

Statistical Analysis .Emphasis should be placed on numerical problems. Significant figures. Accuracy and precision. Errors, systematic and random errors. Propagation of errors. Standard deviation. Coefficient of variation. Confidence limit. Significance test.t-Test, F-Test. Rejection of a result. The least-squares method for deriving calibration graph. Correlation coefficient. Limit of detection.

Sample Preparation for Chromatography. Solid-phase extraction, solid-phase microextraction. Extraction with molecular imprinted polymers.

UNIT II

Chromatography. Theory of Chromatography. Retention time. Capacity factor. Number of theoretical plates, and plate height. Band broadening. Van Deemter equation. Column resolution. *Gas Chromatography*. Instrumentation. Columns. Detection: flame ionisation detector, thermal conductivity detector and mass spectrometric detector.

High-Performance Liquid Chromatography. Instrumentation. Pumping systems. Sample injection system. Columns. Detection: UV-Vis detector, photodiode array detector, fluorescence detector, refractive index detector and mass spectrometric detection. *Capillary Electrophoresis*. Principle, modes of operation, and instrumentation.

UNIT III

Ion Exchange. Cation and anion exchangers. Action of ion exchange resins. Ion exchange equilibria and ion exchange capacity. Strongly and weakly acidic cation exchangers. Strongly and weakly basic anion exchangers. Liquid ion exchangers. Ion chromatography. Conductivity detection using suppressor column. *Solvent Extraction*. The distribution coefficient. Factors favouring solvent extraction. Extraction reagents. Synergetic effects. Ion-pair extraction. Extraction and stripping. Solvent extraction with crown ethers, and factors influencing it.

UNIT IV

Atomic Absorption Spectrometry. Principle. Instrumentation. Flame atomization. Hollow-cathode lamps. Inductively coupled plasma-mass spectrometry. *Electrolytic Methods*.

Fundamentals of the techniques: Voltammetry. Polarography. Differential pulse polarography. Cyclic voltammetry. Anodic stripping analysis.

UNIT V

Acid-Base Titrations. Kjeldahl method for determination of nitrogen. Determination involving acetylation (amino and hydroxyl groups); and oximation (carbonyl group). *Precipitation Titrations.* Argentometric titrations. Mohr titration. Volhard titration. Fajan titration. *Complexometric Titrations.* Titration with EDTA. Indicators for EDTA titrations. Titration methods: direct and back titrations, and displacement methods. Masking and demasking agents, and their use in EDTA titrations. Redox Titrations. Determination of 1,2-diols by periodate oxidation. Karl Fischer titration of water. Determination of DO, BOD and COD.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand analytical chemistry and various techniques.
- Develop an understanding of High Performance Liquid chromatography, Gas Chromatography, its theories and applications.
- Understand Ion exchange Chromatography and Solvent extraction and its theories and applications.
- Develop an understanding of Acid Base Titrations, its types and uses in analytical chemistry.

SUGGESTED READINGS

1. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, Fundamentals of analytical chemistry, Thomson Brooks/Cole, Singapore.
2. D.C. Harris, Quantitative chemical analysis, W.H. Freeman and Co., New York.
3. J.D. Christian, Analytical Chemistry, Wiley, New York.
4. Principles and Practice of Analytical Chemistry, F.W. Fifield and D. Kealey, Blackwell Publishing.
5. S.M. Khopkar, Basic concepts of analytical chemistry, Wiley Eastern, New Delhi.
6. S.M. Khopkar, Analytical chemistry of macrocyclic and supramolecular compounds, Narosa Publishing House, New Delhi.
7. Vogel's Textbook of Quantitative Analysis, revised, J. Bassett, R. C. Denney, G. H. Jeffery and J. Mendham, ELBS.

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<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. II SEM	Elective B	Course MCH 205	Photochemistry	Max: 40	Min: 14

COURSE OBJECTIVE:

- To enrich the students with the understanding of photochemical reactions, their mechanisms and applications.
- To develop an understanding of photochemistry of alkenes, aromatic compounds, carbonyl compounds and miscellaneous reactions and their applications.

UNIT-I

Photochemical Reactions. Interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, actinometry.

UNIT- II

Determination of Reaction Mechanism. Classification, rate constants and life times of reactive energy state determination of rate constants of reactions. Effect of light intensity on the rate of photochemical reactions. Types of photochemical reactions-photo dissociation, gas-phase photolysis.

UNIT III

Photochemistry of Alkene. Intramolecular reactions of the olefinic bond-geometrical isomerism, cyclisation reactions, rearrangement of 1,4- and 1,5-dienes.

Photochemistry of Aromatic Compounds. Isomerisations, additions and substitutions.

UNIT IV

Photochemistry of Carbonyl Compounds. Intramolecular reactions of carbonyl compounds-saturated, cyclic and acyclic, unsaturated and α,β -unsaturated compounds, cyclohexadienones. Intermolecular cycloaddition reactions-dimerisations and oxetane formation.

UNIT V

Miscellaneous Photochemical Reactions. Photo-Fries reactions of annelid's, Photo-Fries rearrangement. Barton reaction. Singlet molecular Oxygen reaction. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand photochemical reactions, mechanisms and applications in organic chemistry
- Develop an understanding of photochemistry of alkenes, aromatic compounds, carbonyl compounds

SUGGESTED READINGS

1. Fundamentals of Photochemistry, K.K.Rohtagi-Mukherji, Wiley-Eastern.
2. Essentials of Molecular Photochemistry, A.Gilbert and Baggott, Blackwell Scientific Publications.
3. Molecular Photochemistry, N.J. Turro, W.A.Benjamin.
4. Introductory Photochemistry, A. Cox and T. Camp, McGraw-Hill. 6. Photochemistry, R.P. Kundall and A. Gilbert, Thomson Nelson.

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<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. III SEM	Core	Course MCH 301	Inorganic Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE:

To provide an overview of group theory, enhance the knowledge of reaction mechanism of transition metals, theory, principle and applications nanomaterials, ESR and *Mössbauer Spectroscopy*.

UNIT-I

Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules. Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations

UNIT-II

Group theory and vibrational Spectroscopy. Group theory to symmetry, shapes and molecular energy level diagrams of molecules like BF_3 , NH_3 (AB_3 type), $[\text{Pt}(\text{NH}_3)_4]^{2+}$, $[\text{Ni}(\text{CN})_4]^{2-}$ (AB_4 type) and $[\text{Co}(\text{NH}_3)_6]^{3+}$ (AB_6 type) molecules. Modes of bonding of ligands such as SCN^- , η -ketoenolate and related ligands, nitrate ion and carboxylates

Application of group theory to Spectroscopy. Use of group theory in predicting IR and Raman active modes in some simple molecules of C_{2v} , C_{3v} and $\text{D}_{\infty h}$ point groups.

UNIT-III

Nanomaterials: Preparative methods: Chemical methods, Solvothermal, Combustion synthesis, Microwave, Co-precipitation, Langmuir Blodgett(L-B) method, Biological methods: Synthesis using microorganisms.

Ceramics- Ceramic Structures, mechanical properties, clay products. Refractories, characterization, properties and applications.

Microscopic Composites dispersion strengthened and particle reinforced composites, macroscopic composites.

UNIT IV

Electron Spin Resonance Spectroscopy. Basic principles, hyperfine and superhyperfine splitting, g value and factors affecting g values, applications to transition metal complexes.

UNIT V

Mössbauer Spectroscopy. Basic principles, spectral parameters and spectrum display. Application of the technique to the studies of (1) bonding and structures of Fe^{+2} and Fe^{+3} compounds including those of intermediate spin, (2) Sn^{+2} and Sn^{+4} compounds -nature of M-L bond, coordination number, structure and (3) detection of oxidation state

COURSE OUTCOME:

By the end of this course student will be able to-

- Gain a thorough knowledge about Group theory and applications to molecules.
- Build the concept of Electron Spin Resonance and Mossbauer Spectroscopy and their application in structure elucidation.

SUGGESTED READINGS

1. Jag Mohan. (2018). Organic Spectroscopy: Principle and Applications (II Edition). New Delhi: Narose Publishing House.
2. Kemp, W. (2017). Organic Spectroscopy (III Edition). New York: Palgrave Macmillan.
3. Sharma, Y. R. (2013). Elementary Organic Spectroscopy: Principles and Chemical Applications (Revised V Edition). New Delhi: S. Chand & Company Limited.
4. Silverstein, R. M., Webster, F. X., & Kiemle, D. (2014). Spectroscopy of Organic Compounds (VIII Edition). New York: John Wiley & Sons.
5. Levine, I. N. (2013). Quantum Chemistry (VII Edition). New Delhi: Pearson Education Pvt. Ltd.
6. Drago, R.S. (2012). Physical Methods in Inorganic Chemistry. New York: East- West Press Pvt. Ltd.
7. Banwell.,(2017). Fundamentals of Molecular & Spectroscopy (IV Edition), McGraw-Hill Education (India) Pvt. Limited

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<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. III SEM	Core	Course MCH 302	Physical Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE:

To understand the concept of Molecular orbital theory, Crystal defects, *Electronic Properties and Band Theory*.

UNIT I

Electronic Structure of Atoms. Electronic configuration, Russell-Saunders terms and coupling scheme, Slater parameters, magnetic effects. Zeeman splitting; virial theorem.

UNIT II

Molecular Orbital Theory. Hückel theory of conjugated systems, bond order and charge density calculations. Applications to ethylene, butadiene, and cyclobutadiene. Introduction to extended Hückel theory.

UNIT III

Homogeneous Catalysis. Stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerisation of olefins.

Heterogenous Catalysis. Thermodynamics of active centres, mechanism of heterogenous catalysis; structural promotion and structural modification.

UNIT IV

Crystal Defects. Perfect and imperfect crystals, stoichiometric and non-stoichiometric defects. Intrinsic and extrinsic defects, point defects, line and plane defects; Schottky and Frenkel defects.

Solid State Reactions. General principles, coprecipitation as a precursor to solid state reactions, factors affecting solid state reactions.

UNIT V

Electronic Properties and Band Theory. Metals, insulators and semiconductors. Electronic structure of solids Band theory; band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, superconductors.

Course Outcome:

By the end of this course student will be able to-

- Develop concepts of Electronic Structure of Atoms and Molecular Orbital Theory and their applications.
- Enhance the knowledge about Homogenous and Heterogenous Catalysis.
- Develop an understanding of the Crystal defects and Solid state Reactions
- Build concepts of Electronic Properties and Band theory, types and applications on insulators, semiconductors and superconductors.

SUGGESTED READINGS

1. Bahl, A., Bahl, B. S., & Tuli, G. D, (2014). Essentials of Physical Chemistry (VEdition). New Delhi: S. Chand & Company.
2. Puri, B.R., Sharma, L.R., & Pathania, M.S. (2015). Elements of Physical Chemistry. Jalandhar: Vishal Publishing House.
3. Laidler, K. J. (2004). Chemical Kinetics (III Edition). New Delhi: Pearson Education Publishing. Indian Branch.
4. Gurdeep Raj, Chemical Kinetics, Goel Publishing House.
5. A.A.Frost and R.G.Pearson, Kinetics and Mechanism, Wiley Eastern, Pvt. Ltd.
6. Emmet, P. H. (1954). Catalysis (Vol I and II). Reinhold

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<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. III SEM	Core	Course MCH 303	Spectroscopy III	Max: 40	Min: 14

COURSE OBJECTIVE:

To understand the principle, theories, instrumentation and applications of C^{13} NMR, Mass, Electron diffraction and neutron diffraction spectroscopic techniques

UNIT I

^{13}C -NMR Spectroscopy General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), wide band H-decoupled and off-resonance H-decoupled spectra. Calculation of chemical shift values for alkanes and substituted benzene. Two dimension NMR spectroscopy. COSY, and DEPT techniques. *Conjoint Spectroscopy Problems*. Application of UV, IR, Raman, NMR and Mass spectrometry for elucidation of structure of organic compounds.

UNIT II

Mass Spectrometry-Part I. Ion production, electron ionisation (EI), chemical ionisation (CI), field desorption (FD), field ionisation (FI), and fast atom bombardment (FAB). Atmospheric pressure ionisation techniques. Electrospray ionisation, and atmospheric pressure chemical ionisation. Thermospray ionisation. Matrix assisted laser desorption ionisation (MALDI). Mass analysers. Magnetic sector analysers. Quadrupolar analysers, ion trap, time-of-flight (TOF), ion cyclotron resonance (ICR). Electron multiplier. Tandem mass spectrometry (MS/MS).

UNIT III

Mass Spectrometry-Part II. Isotopic abundance. Electron ionisation and fragmentation (positive ions). Molecular ion peak, metastable peak. McLafferty rearrangement. Nitrogen rule. Parity rule. Mass spectral fragmentation of organic compounds containing common functional groups (alkanes, alkenes, alkynes, halo-compounds, alcohols, amines, carbonyl compounds, aromatic compounds).

High resolution mass spectrometry. Interpretation of mass spectra. Problems based on mass spectrometry of organic compounds.

UNIT IV

X-ray Diffraction. Bragg condition, Miller indices, Laue method, Bragg method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, structure factor and its relation to intensity and electron density. Description of the procedure for an X-ray structure analysis.

UNIT V

Electron Diffraction. Scattering intensity vs. scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

Neutron Diffraction. Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cell.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand C13 NMR and its application in structure elucidation.
- Build concepts of Mass spectrometry, its techniques, applications and interpretation of spectra.
- Understand and apply the concepts of X Ray, Electron and Neutron diffraction, its types and applications for structure elucidation of organic compounds
- Develop an understanding of Conjoint Spectroscopy for elucidation of structure of organic compounds using UV, IR, Raman, NMR and Mass Spectroscopy.

SUGGESTED READINGS

10. Modern Spectroscopy, J.M. Hollas, John Wiley.
11. Applied Electron Spectroscopy for Chemical Analysis Ed. H. Windawi and F.L. Ho, Wiley Interscience.
12. Physical Methods in Chemistry, R.S. Drago, Saunders College.
13. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill.
14. Basic Principles of Spectroscopy, R. Chang, McGraw Hill.
15. Introduction to Photoelectron Spectroscopy: P. K. Ghosh, John Wiley.
16. Macromolecules: Structure and Function, F. Wold, Prentice Hall.
17. Fundamentals of molecular spectroscopy, C.N. Banwell, Tata McGraw-Hill, New Delhi.
18. Instrumental Methods of Analysis, Willard, Meritt and Dean.

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. III SEM	Elective A	Course MCH 304	Medicinal Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE

- To understand the basics of Medicinal chemistry, drug targets, drug metabolism, membrane and receptors in drug delivery process.
- To apply the various theories of Drugs, their mechanism and mode of action for various kinds of drugs

UNIT I

Structure and activity. Relationship between chemical structure and biological activity (SAR). Receptor Site Theory. Approaches to drug design. Introduction to combinatorial synthesis in drug discovery. Factors affecting bioactivity. QSAR-Free-Wilson analysis, Hansch analysis, relationship between Free-Wilson analysis and Hansch analysis.

UNIT II

Pharmacodynamics. Introduction, elementary treatment of enzymes stimulation, enzyme inhibition, sulfonamides, membrane active drugs, drug metabolism, xenobiotics, biotransformation, significance of drug metabolism in medicinal chemistry.

UNIT III

Antibiotics and antibacterials. Introduction, Antibiotic β -Lactam type - Penicillins, Cephalosporins, Antitubercular . Streptomycin, Broad spectrum antibiotics .Tetracyclines, Anticancer – Dactinomycin (Actinomycin D)

UNIT IV

Antifungal polyenes, Antibacterials. Ciprofloxacin, Norfloxacin, Antiviral. Acyclovir Antimalarials. Chemotherapy of malaria. SAR.Chloroquine, Chloroguanide and Mefloquine

UNIT V

Non-steroidal Anti-inflammatory Drugs. Diclofenac Sodium, Ibuprofen and Netopam Antihistaminic and antiasthmatic agents: Terfenadine, Cinnarizine, Salbutamol and Beclomethasone dipropionate.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand Medicinal Chemistry and its application in pharmaceutical chemistry.
- Develop an understanding of Structure and Reactivity, Pharmacodynamics in Drug Design, Metabolism and Development.
- Enhance the knowledge about Antibiotics, Antibacterials, Antifungals and NSA Drugs their structure, synthesis, mode of action, advantages and disadvantages.

SUGGESTED READINGS

1. Ahluwalia, V. K. (2012). Green Chemistry-Environmentally Benign Reactions. New Delhi: Ane Books Pvt Ltd.
2. Ghose, J. (2012). A Text book of Pharmaceutical Chemistry. New Delhi: S. Chand Pub Ltd.
3. Ilango, K., & Valentina, P. (2017). Text Book of Medicinal Chemistry. Vol II. Chennai: Keerthi Publishers.
4. Ashutosh Kar, (2018). Medicinal Chemistry (III Edition). New Delhi: New Age International Publishers. 5. Stanley E. Manahan, (2006). Green Chemistry and the Ten Commandments of Sustainability (II Edition). Columbia, Missouri U.S.A: ChemChar Research. Inc Publishers Columbia.
6. Chatterjea, M. N., & Shinde, R. (2012). Textbook of Medicinal Biochemistry. New Delhi: Jaypee Brothers. Medical Publishers (P) Ltd. 7. G.L. Patrick, (2013). Introduction to Medicinal Chemistry (I Edition). UK: Oxford University Pre

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<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. III SEM	Elective B	Course MCH 304	Chemistry of Natural Products	Max: 40	Min: 14

COURSE OBJECTIVE

To understand the importance of natural products, their structure, synthesis and applications.

UNIT I

Terpenoids. General methods of structure elucidation. Isoprene rule. Structure determination, stereochemistry, and synthesis of the following representative molecules: citral, geraniol, α -terpineol, menthol, α -pinene, camphor, and abietic acid. Biosynthesis of terpenoids.

UNIT II

Alkaloids. General methods of structure elucidation. Structure determination, stereochemistry, and synthesis of the following representative molecules: ephedrine, nicotine, atropine, quinine and morphine. Biosynthesis of alkaloids.

UNIT III

Steroids. Structure elucidation, stereochemistry and chemical synthesis of cholesterol, bile acids, androsterone, testosterone, estrone, progesterone and aldosterone. Biosynthesis of steroids.

UNIT IV

Plant Pigments. *Carotenoids.* Structure and synthesis of β -carotene. *Flavonoids.* Nature, general methods for structure elucidation and synthesis of anthocyanins and flavones. Structure and synthesis of cyanidin chloride, cyanin, flavone, flavonol and quercetin. Biosynthesis of flavonoids. *Chlorophyll.* Chemistry of chlorophyll.

UNIT V

Vitamins and Antibiotics. *Vitamins.* Structure and synthesis of vitamin B₁ (thiamine), B₂ (riboflavin) and B₆ (pyridoxine). Chemistry of Vitamin B₁₂. *Antibiotics.* Structure and synthesis of penicillins and chloramphenicol.

Course Outcome:

By the end of this course the student will be able to

- Understand Chemistry of Natural Products and their application in pharmaceutical chemistry.
- Develop an understanding of Alkaloids, Steroids, Carotenoids, Vitamins, Flavonoids and Antibiotics, their structure, synthesis and applications.

SUGGESTED READINGS:

1. Chatwal, G. R. (2015). Organic Chemistry of Natural Products Vol. II. New Delhi: Himalaya Publishing House.
2. Finar, I. L. (2013). Organic Chemistry Vol. II: Stereochemistry and the Chemistry of Natural Products (V Edition). New Delhi: Pearson Education, Ltd.
3. Chatwal, G. R. (2015). Organic Chemistry of Natural Products. Vol. I. New Delhi: Himalaya Publishing House.
4. Saluja, M. P., Raj Kumar & Anuja Agarwal (2017). Advanced Natural Products (Revised IV Edition). Meerut: Krishna Prakashan Media (P) Ltd.

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. III SEM	Elective C	Course MCH 304	Polymers	Max: 40	Min: 14

COURSE OBJECTIVE:

- To enable the student to get knowledge about the basic concepts of polymerization, and classification.
- To provide knowledge about properties, structure, processing techniques and applications of commercial polymers.

UNIT I

Basics of Polymers. Repeating units, degree of polymerisation, linear, branched and network polymers. Classification of polymers. Addition, radical, ionic, coordination and condensation polymerisation; their mechanism and examples.

Polymerisation conditions and polymer reactions. Polymerisation in homogeneous and heterogeneous systems.

UNIT II

Polymer Characterisation. Significance of molecular weight of polymer. Polydispersive average molecular weight. Number, weight and viscosity average weights. Measurement of molecular weights. End group, viscosity, light scattering, osmotic and ultracentrifugation methods. Chemical and spectroscopic analysis of polymers. X-Ray diffraction study. Thermal analysis, tensile strength, fatigue, impact. Tear resistance. Hardness and abrasion resistance.

UNIT III

Structure and Properties. Configuration of polymer chains. Crystal structure of polymers. Morphology of crystalline polymers. Polymer structure and physical properties; crystalline melting point T_m , melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g relationship between T_m and T_g , effects of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilization.

UNIT IV

Polymer Processing. Plastics, elastomers and fibres. Compounding. Processing techniques, Calendering, die casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, foaming, reinforcing and fibre spinning.

UNIT V

Properties of Polymers. Properties of polyethylene, polyvinyl chloride, polyamides, polyesters, phenolic resins, epoxy resins and silicone polymers. Functional polymers. Fire retarding polymers, and electrically conducting polymers. Biomedical polymers. Contact lens, dental polymers, artificial heart, kidney, skin and blood cells.

COURSE OBJECTIVE:

By the end of this course student will be able to-

- Create an understanding Polymer Chemistry and its industrial applications.
- Develop an understanding of Polymer basics and characterization, its structure and properties.
- Understand the Polymer processing and their properties and applications in biomedical field.

SUGGESTED READINGS

1. Billmeyer, F. W. (2003). Text Book of Polymer Science (III Edition). New York: John Wiley.
2. Alcock, H. R., Lampe, F. W., & Mark, J. E. (2003). Contemporary Polymer Chemistry (III Edition). NJ: Prentice Hall Englewood Cliffs.
3. Flory, P. J. (1953). Principles of Polymer Chemistry. New York: Cornell University Press.
4. Odian, G. (2004). Principles of Polymerization (IV Edition). New York: John Wiley & Sons.
5. Textbook of Polymer Science, F.W. Billmeyer, Jr., Wiley.
6. Polymer Science, V.R. Gwariker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
7. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and R.M. Ottanbrite.
8. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
9. Physics and Chemistry of Polymers, J.M.G. Cowie, Blackie Academic and Professional.

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. IV SEM	Core	Course MCH 401	Inorganic Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE: To enable the students in understanding various Aspects of Bioinorganic chemistry, Electron Transfer in Biology, organic reagent in organic chemistry, Photosystems and energy transfer concept

Unit-I

Organic Reagents in Inorganic Chemistry: Chelation, factors determining the stability of chelates (effect of ring size, oxidation state of the metal, coordination number of the metal); Use of the following reagents in analysis:

- (a) Dimethylglyoxime (in analytical chemistry)
- (b) EDTA (in analytical chemistry)
- (c) 8-Hydroxyquinoline (in analytical chemistry)
- (d) 1,10-Phenanthroline (in analytical chemistry)
- (e) Thiosemicarbazones (in analytical chemistry)
- (f) Dithiazone (in analytical chemistry)

UNIT II

Bioinorganic Chemistry. Metal containing enzymes: Carboxypeptidase-A, Carbonic anhydrase, arginase, urease, DNA polymerase, phosphoglucosyltransferase (glucose storage): structure and reactivity

UNIT III

Bioinorganic Chemistry: Metal complexes in transmission of energy: Chlorophylls, photosystem-I and photosystem-II in cleavage of water, model systems.

UNIT IV

/Electron Transfer in Biology: Structure and function of metalloproteins in electron transport processes-cytochromes and iron-sulphur proteins. Nitrogenase: Biological nitrogen fixation, molybdenum nitrogenase-structure and function.

UNIT V

Transport and Storage of Dioxygen Structure and function of haemoglobin, myoglobin, hemocyanin and hemerythrin. Poisoning towards haemoglobin and myoglobin.

COUSE OUTCOME:

By the end of this course student will be able to-

- Gain a thorough knowledge about Organic Reagents in Inorganic Chemistry, their structure and applications
- Develop the concept of Bioinorganic Chemistry, metal containing enzymes and metal complexes in energy transmission.
- Build the concept of Electron transfer in Biology, transport and storage of dioxygen.

SUGGESTED READINGS

1. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
2. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
3. Inorganic Biochemistry vols I and II. ed. G.L. Eichturn, Elsevier.
4. Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley, Environmental Chemistry, S. E. Manahan, Lewis Publishers.

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. IV SEM	Core	Course MCH 402	Organic synthesis strategies	Max: 40	Min: 14

COURSE OBJECTIVE

- To enable students to know various strategies used in retro synthetic analysis, chemistry of various organic reagents and the chemistry of Oxidation and Reduction reactions
- To understand basics of asymmetric synthesis, chemistry of various reagents, reaction and mechanism of selected named reactions, the chemistry of protecting and deprotecting groups and synthesis of selected drug molecules.

UNIT I

Oxidation. Oxidation of carbon carbon double bond. Perhydroxylation, potassium permanganate, osmium tetroxide, iodine together with silver carboxylates, ozonolysis. Enantioselective epoxidation of allylic alcohols (Sharpless epoxidation). Oxidation of alcohols. Chromic acid, chromium (VI) oxide-pyridine complexes, manganese (IV) oxide, silver carbonate, oxidation via alkoxy sulphonium salts. Baeyer-Villiger oxidation of ketones. Oxidation with ruthenium tetroxide, thallium(III) nitrate and iodobenzene diacetate.

UNIT II

Reduction. Catalytic hydrogenation (homogeneous and heterogeneous). Stereochemistry and mechanism, selectivity of reduction. Reduction by dissolving metals. Metal and acid, metal and alcohol, metal and ammonia.

Reduction by hydride-transfer reagents. Aluminium alkoxides, lithium aluminium hydride, sodium borohydride, lithium hydrido-alkoxyaluminates. Wolff-Kishner reduction. Reduction with di-imide

UNIT III

Designing organic synthesis. The Disconnection Approach. Basic principles, synthons, functional group interconversions. Order of events in organic synthesis. One group CX disconnections and two group CX disconnections. Chemoselectivity. Reversal of polarity (umpolung). Amine synthesis

UNIT IV Organic reagent

Organic Reagents: Reagents in organic synthesis: Wilkinson catalyst, Lithium dialkylcuprates (Gilman's reagents), Lithium diisopropylamide (LDA), 1,3-Dithiane (Umpolung) Dicyclohexylcarbodiimide (DCC), and Trimethylsilyliodide, DDQ, SeO₂, Baker yeast, Tri-nbutyltinhydride, Nickel tetracarbonyl, Trimethylchlorosilane

UNIT V

Rearrangement General mechanistic considerations-nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Backmann, Hofmann, Curtius, Schmidt, Benzidine, Baeyer-Villiger, Shapiro reaction, Witting rearrangement and Stevens rearrangement.

COURSE OUTCOME

By the end of this course student will be able to-

- Create an understanding Organic Synthesis Strategies and its application.
- Gain knowledge about concept of Oxidation, Reduction and Rearrangement reactions and their applications to some known reactions.
- Develop an understanding Disconnection approach, types and chemoselectivity.

SUGGESTED READINGS

1. Warren, S. (2010). Organic Synthesis the Disconnection approach, Wiley and sons,
2. Renuga, S. (2016). Name reactions and reagents in organic synthesis, Vishal Publishing Co. Jalandhar-Delhi.
3. Nasir Hussain and Saba Khan, (2016). Reactions and Reagents, Himanshu Publications, New Delhi.
4. Clayden, J., Greeves, N. & Warren, S. (2012). Organic Chemistry (II Edition). Oxford University Press, Oxford.
5. Sanyal, S. N. (2014). Reactions, Rearrangements and Reagents (IV Edition). New Delhi: Bharathi Bhawan (Publishers and Distributors).
6. Smith, M. B. (2015). March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure (VII Edition). New Jersey: John Wiley & Sons, Inc., Hoboken.
6. Warren, S., & Wyatt, P. (2008). Organic Synthesis: The Disconnection Approach (II Edition). John Wiley & Sons Ltd., Chichester.

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title</i> (<i>Theory/Practical</i>)	<i>Marks</i>	
M.Sc. IV SEM	Departmental Elective	Course MCH 403 A	Environmental Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE:

To provide an overview of water, air, soil, radioactive and noise pollution including methods for prevention of pollution and its control measures.

Unit I

Environment Introduction. Composition of atmosphere, vertical temperature, temperature inversion, heat budget of the earth, atmospheric system, vertical stability atmosphere, Biochemical cycles of C,N, P, S and O. Biodistribution of elements.

Hydrosphere Chemical composition of water bodies-lakes, streams, rivers and wet lands etc. Hydrological cycle Aquatic pollution – Inorganic, organic, pesticide, agriculture, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and microorganisms. Water quality standards. Analytical methods of measuring BOD, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chlorine demand. Purification and treatment of water.

Unit II

Soils-Composition, micro and macro nutrients, pollution – fertilizers, pesticides, plastics and metals. Waste treatment.

Atmosphere Chemical composition of atmosphere – particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N,

C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

Unit III**Industrial Pollution**

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Environmental disasters – Chernobyl, Three mile island, Seveso and Minamata disasters, Japan tsunami.

Unit IV

Environmental Toxicology Toxic heavy metals :Mercury, lead, arsenic and cadmium. Causes of toxicity. Bioaccumulation, sources of heavy metals. Chemical speciation of Hg, Pb, As, and Cd. Biochemical and damaging effects.

Toxic Organic Compound : Pesticides, classification, properties and uses of organochlorine and ionospheres pesticides detection and damaging effects.

Unit-V

Aquatic Chemistry and Water Pollution. Redox chemistry in natural waters. Dissolved oxygen, biological oxygen demand, chemical oxygen demand, determination of DO, BOD and COD. Aerobic and anaerobic reactions of organic sulphur and nitrogen compounds in water acid-base chemistry of fresh water and sea water. Aluminum, nitrate and fluoride in water. Petrification. Sources of water pollution. Treatment of waste and sewage. Purification of drinking water, techniques of purification and disinfection.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand Environmental Chemistry and its concepts.
 - Build concepts of Hydrosphere, Atmosphere and Soil, their composition, and side effects pollution.
 - Understand and apply the concepts industrial pollution and study of some famous environmental disasters.
 - Understand and apply the concepts Water pollution, purification and treatment and study of some prime pollutants.
 - Develop an understanding of environmental toxicology and some toxic Organic Compounds.
1. Environmental Chemistry, Colin Baird, W.H. Freeman Co. New York, 1998.
 2. Chemistry of Atmospheres, R.P. Wayne, Oxford.
 3. Environment Chemistry, A.K. De, Wiley Eastern, 2004.
 4. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
 5. Introduction to atmospheric Chemistry, P.V. Hobbs, Cambridge.
 6. Environmental Chemistry, S.E. Manahan, Lewis Publishers.
 7. Environmental chemistry, Sharma and Kaur, Krishna Publishers.
 8. Environmental Chemistry, Analysis, S.M. Khopkar, Wiley Eastern.
 9. Standard Method of Chemical Analysis, F.J.Welcher Vol.III, VanNostr and ReinholdCo.
 10. Environmental Toxicology, Ed.J.Rose, Gordon and Breach Science Publication. 7. Environmental Chemistry, C. Baird, W.H.Freeman.

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. IV SEM	Departmental Elective	Course MCH 403 B	Chemistry of Materials	Max: 40	Min: 14

COURSE OBJECTIVE: To bridge the gap between fundamental ideas of chemistry to modern research and industry-related topics.

UNIT I

Ceramics, Composites and Nanomaterials. Ceramic structures, mechanical properties, clay products. Refractories, characterization, properties and applications. Microscopic composites, dispersion-strengthened and particle-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, properties and applications.

UNIT II

Liquid Crystals. Thermotropic liquid crystals, positional order, bond orientational order, nematic and smectic mesophases. Molecular arrangement in smectic A and smectic C phases, optical properties of liquid crystals. Dielectric susceptibility and dielectric constants. Lyotropic phases and their description of ordering in liquid crystals.

UNIT III

Ionic Conductors. Types of ionic conductors, mechanism of ionic conduction, interstitial jumps (Frenkel); vacancy mechanism, diffusion superionic conductors, phase transitions and mechanism of conduction in superionic conductors. Examples and applications of ionic conductors.

UNIT IV

High T_c Materials. High T_c superconductivity. Preparation and characterization of 1-2-3 and 2-1-4 materials. Normal state properties, anisotropy, temperature dependence of electrical resistance, and optical phonon modes. Superconducting state; heat capacity; coherence length, elastic constants, microwave absorption-pairing and multigap structure in high T_c materials. Applications of high T_c materials.

UNIT V

Organic Solids, Fullerenes, Molecular Devices. Conducting organics, organic superconductors, magnetism in organic materials. Fullerenes, doped, fullerenes as superconductors. Molecular rectifiers and transistors, artificial photosynthetic devices, optical storage memory and switches, sensors. Non-linear optical materials, non-linear optical effects. Molecular hyperpolarisability.

Course Outcome:

By the end of this course student will be able to-

- Develop an understanding Chemistry of Materials and its application in chemistry.
- Develop an understanding of Ceramics, Composites and Nanomaterials, their structure, characterization, properties and applications.
- Understand and apply the concepts Liquid Crystals and Ionic conductors, their structure, types, properties and applications in wide variety of chemistry, physics and allied fields.
- Build the concept of Superconductors and its indepth study for understanding of their possible applications.
- Build concepts of Organic solids, Fullerenes and Molecular Devices and its applications.

SUGGESTED READING

1. Materials Science and Engineering: An Introduction (Hardcover) by William D. Callister Jr.
2. Introduction to Materials Science for Engineers by James Shackelford
3. Foundations of Materials Science and Engineering by William Smith
4. The Science and Engineering of Materials by Donald Askeland and Wendelin Wright
5. Material Science and Metallurgy by OP Khanna

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. IV SEM	Open Elective	Course MCH 404 A	Biochemistry	Max: 40	Min: 14

COURSE OBJECTIVE: To provide a comprehensive introduction to biochemistry and to learn the chemistry of enzymes, structures of nucleic acids and biosynthesis of proteins.

UNIT-I

Carbohydrates: Types of naturally occurring sugars: Deoxy-sugars, amino sugars, branched chain sugars. General methods of structure and ring size determination with particular reference to maltose, lactose, sucrose, pectin, starch and cellulose, photosynthesis of carbohydrates, metabolism of glucose, Glycoside- (amygdalin).

UNIT-II

Amino acid, peptides and proteins: General methods of peptide synthesis, sequence determination. Chemistry of insulin and oxytocin. Purines and nucleic acid. Chemistry of uric acid, adenine, protein synthesis.

UNIT-III

Vitamins: A general study, detailed study of chemistry of thiamine (Vitamin B1), Ascorbic acid (Vitamin C), Pantothenic acid, biotin (Vitamin H), α -tocopherol (Vitamin E), Biological importance of vitamins.

UNIT-IV

Enzymes: Nomenclature and classification, extraction and purification, Remarkable properties of enzymes like catalytic power, specificity and regulation, Proximity effects and molecular adaptation, Chemical and biological catalysis. Mechanism of enzyme action: Transition state theory, orientation and steric effect, acid base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms (chymotrypsin, ribo nuclease, lysozyme and carboxypeptidase A). Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors affinity labeling and enzyme modification by site directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

UNIT-V

(A) Kinds of reactions catalyzed by Enzymes: Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Transfer of sulphate addition and elimination reactions, enolic intermediates in isomerization reactions, β - cleavage and condensation, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation reactions.

(B) Coenzyme Chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate

pyridoxal phosphate, NAD⁺, NADP⁺, FMN, FAD, Lipoic acid, vitamin B12. Mechanisms of reactions catalyzed by the above cofactors.

COURSE OUTCOME:

By the end of this course student will be able to-

- Understand Biochemistry and its application in chemistry.
- Gain knowledge about concept of Carbohydrates, Amino Acids, Vitamins and enzymes their structure, types, properties, metabolism, synthesis and uses in the human body.

SUGGESTED READINGS

1. Biochemistry, D. Voet and J.G. Voet, John Wiley.
2. Principles of Biochemistry, A.L. Lehninger, D.L. Nelson and M.M. Cox, CBS Publishers, Delhi.
3. Immobilized Enzymes: An Introduction and Applications in Biotechnology, Michael D. Trevan, John Wiley.

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. IV SEM	Open Elective	Course MCH 404 B	Bioorganic Chemistry	Max: 40	Min: 14

COURSE OBJECTIVE

To Understand reactions Catalyzed by Enzymes, chemical strategies and mechanisms behind enzyme catalysis, enzyme models and Biotechnological Application of enzymes.

Unit-I

Introduction :Basic Consideration, Proximity effects and molecular adoption. Enzymes: Introduction, Chemical and Biological catalysis, remarkable properties of enzymes, Nomenclature and classification, concept and identification of active site by use of inhibitors, reversible & irreversible inhibition.

Unit-II

Kinds of Reactions Catalyzed by Enzymes: B-cleavage and consideration, some isomerization and rearrangement reactions. Enzyme catalyzed carboxylation and decarboxylation. Mechanism of Enzyme action: Transition state theory, Orientation and steric effect, acid-base catalysis, covalent catalysis. Co-Enzyme Chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes, Structure and biological functions of coenzyme A.

Unit-III

Enzyme Models :Host guest chemistry, Chiral recognition and catalysis, molecular recognition, molecular asymmetry and prochirality, Biomimetic chemistry, crown ethers, cryptates, cyclodextrins, cyclodextrin based enzyme models, Calixarenes, ionophores, micelles synthetic enzyme or synzymes.

Unit-IV

Biotechnological Application of enzymes: Large scale production and purification of enzymes, techniques and methods of immobilization of enzyme activity, application of immobilized enzymes, effect of immobilization on Enzyme activity, application of immobilized enzymes. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

Unit-V

Metalloenzymes Copper enzymes, superoxide dismutase, cytochrome oxidase and ceruloplasmin; Coenzymes; Molybdenum enzyme: xanthine oxidase; Zinc enzymes: carbonic anhydrase, carboxy peptidase and interchangeability of zinc and cobalt in enzymes; Vitamin B12 and B12 coenzymes; Iron storage, transport, biomineralization and siderophores, ferritin and transferrins..

Course Outcome:

By the end of this course student will be able to-

- Understand of Bioorganic chemistry and its applications.
- Gain knowledge about Enzymes, their nomenclature, classification, properties,, models and biotechnological and clinical applications.
- Apply knowledge of organic and bioorganic chemistry to predict chemical properties and reactivity in chemical and biological contexts and propose mechanistic hypotheses for reactions.

SUGGESTED READINGS

1. Bioorganic, BioInorganic and Supramolecular Chemistry by P. S. Kalsi and J. P. Kalsi
2. Structure and Mechanism in Protein Science: A Guide to Enzyme Catalysis and Protein Folding” by A R Fersht and W H Freeman.
3. “Bioorganic Chemistry” by H Dugas.
4. Bioorganic Chemistry: A Chemical Approach to Enzyme Action (Springer Advanced Texts in Chemistry)” by Hermann Dugas

St. Aloysius (Autonomous) College, Jabalpur

Department of Chemistry

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. I SEM	Practical	Course MCH 106	Inorganic Chemistry	Max: 50	Min: 18

Qualitative analysis:

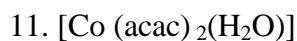
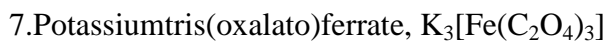
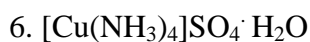
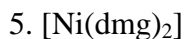
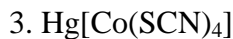
1. To identify the given cation, anion and interfering radicals (total six including one interfering radical) from the given inorganic mixture.

Chromatography

1. Separation of cations and anions by Paper Chromatography
2. Separation of cations and anions by Column Chromatography; Ion exchange

Synthesis:

Preparation of selected inorganic compounds and their studies by measurements of decomposition temperature, molar conductance, I.R., electronic spectra, and magnetic susceptibility measurements.



14. Potassium tris(oxalato)ferrate, $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$ and determination of oxalate using permanganate.

Interpretation of IR and Electronic Spectra of some known compounds

St. Aloysius (Autonomous) College, Jabalpur

Department of Chemistry

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. I SEM	Practical	Course MCH 107	Physical Chemistry	Max: 50	Min: 18

Maximum Marks: 50

Minimum Marks: 20

Adsorption

1. To study surface tension -concentration relationship for solutions (Gibbs equation).

Phase Equilibria

2. To construct the phase diagram for three component system (e.g., chloroform-acetic acid-water). *Polarimetry*
3. To calculate specific rotation of sucrose
4. Enzyme kinetics -inversion of sucrose

Chemical Kinetics

5. Determine the rate constant of hydrolysis of an ester as methyl acetate catalysed by an acid
Determine also the energy of activation of the reaction
6. Determination of the velocity constant of hydrolysis of an ester and to study the effect of change of concentration on it.

Adsorption

7. To study the adsorption of oxalic acid on charcoal and to prove the validity of Freundlich adsorption isotherm.
8. To study the adsorption of oxalic acid on charcoal and to prove the validity of Langmuir's adsorption isotherm.

Electronics

9. To study the variation of thermo emf with the temperature for the copper-iron thermocouple.
10. To study forward and reverse characteristics of Si and Ge semiconductor diode
11. To observe the wave form of (i) a.c. mains supply and (ii) an oscillator using cathode ray oscilloscope

pH metry

12. To determine the strength of unknown (strong) acid pHmetrically using standard alkali solution (strong).

Conductometry

13. To determine the strength of unknown (strong) acid conductometrically using standard alkali solution (strong).
14. To determine the basicity of an acid.

Potentiometry

15. To determine the strength of unknown (strong) acid potentiometrically using standard alkali solution (strong).

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. II SEM	Practical	Course MCH 206	Organic Chemistry	Max: 40	Min: 14

Maximum Marks: 50**Minimum Marks: 20****Analysis**

Separation, purification and identification of compounds of binary mixture (one solid and one liquid/solid) using chemical separation and sublimation/distillation, etc. Their analysis by semi-micro chemical tests and spot tests. IR spectra to be used for functional group identification. Preparation of one derivative of each compound. Emphasis should be placed on physical principles, reaction chemistry and the technique involved in analysis.

Organic Synthesis

Aromatic electrophilic substitutions:

1. Synthesis of m-dinitrobenzene from nitrobenzene
2. Synthesis of 2,4-dinitro-1-chlorobenzene from chlorobenzene
3. Synthesis of 4-bromoaniline from acetanilide

Reduction reaction:

Synthesis of m-nitroaniline from m-dinitrobenzene

Oxidation reaction

1. Synthesis of 9,10-anthraquinone by oxidation of anthracene by chromium trioxide
2. Synthesis of 4-nitrobenzaldehyde by oxidation of 4-nitrotoluene by chromium trioxide

Cannizzaro reaction

1. Synthesis of benzyl alcohol from benzaldehyde

Claisen-Schmidt reaction:

2. Synthesis of dibenzylideneacetone (1,5-diphenylpenta-1,4-dien-3-one) from acetone and benzaldehyde

Sandmeyer reaction:

3. Synthesis of 2-chlorobenzoic acid from anthranilic acid

Methylation:

4. Synthesis of methyl 2-naphthyl ether (2-methoxynaphthalene, nerolin) by methylation of 2-naphthol by dimethyl sulphate.

Purification of compounds by TLC and column chromatography

St. Aloysius (Autonomous) College, Jabalpur

Department of Chemistry

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. II SEM	Practical	Course MCH 207	Inorganic Chemistry	Max: 50	Min: 18

Maximum Marks: 50

Minimum Marks: 20

Gravimetric Estimation (any two experiments):

Estimate mixture of 2 metal ions (Copper and Zinc)

Spectrophotometric Determination

1. Determination of molecular composition of ferric salicylate /iron-phenanthroline/iron-dipyridyl complex by Job's method of continuous variation
2. Determination of the pH of a given solution by spectrophotometry using methyl red indicator

Synthesis.

1. Aquabis(acetylacetonato)nitrosylchromium(I), $[\text{Cr}(\text{NO})(\text{acac})_2(\text{H}_2\text{O})]$
2. cis-Bis(glycinato)copper(II) and trans-Bis(glycinato)copper(II)
3. Preparation of Zn, Cd and Hg thiocyanates from their respective chlorides
4. Bis(benzoylacetonato)copper(II)
5. Bis (acetylacetonato)oxovanadium(IV), $[\text{VO}(\text{acac})_2]$
6. $[\text{MoO}_2(\text{acac})_2]$
7. Hexaamminenickel(II)tetrafluoroborate, $[\text{Ni}(\text{NH}_3)_6](\text{BF}_4)_2$ and determination of nickel content gravimetrically.
8. Potassium tris(oxalato)ferrate, $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$ and determination of oxalate using permanganate.
9. Preparation of N,N-bis(salicylaldehyde)ethylenediamine $[\text{salenH}_2]$, $\text{Co}(\text{salen})$

Interpretation of ESR, NMR and Thermogravimetric pre-recorded results of known compounds

Pre-recorded spectrum/data shall be provided for their interpretation leading to structure determination of metal ion complexes with organic ligands

St. Aloysius (Autonomous) College, Jabalpur

Department of Chemistry

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. III SEM	Practical	Course MCH 305	Organic Chemistry	Max: 50	Min: 18

Maximum Marks: 50

Minimum Marks: 20

Analysis

1. Estimation of protein by Lowry's method.
2. Estimation of carbohydrate by Anthrone's method
3. Isolation of caffeine and alkaloids from tea.
4. To determine the iodine value of the given oil or fat
5. To determine the Saponification value of the given oil or fat
6. Estimation of Ascorbic Acid i.e. vitamin C.
7. Estimation of Amino acid by Sorenson's method
8. Spectrophotometric estimation of Glucose with the help of Fehling solution

Multi Step Synthesis

1. Benzoin- benzyl- benzilic acid
2. Benzophenone –benzpinacole- benzpinacolone
3. Ethyl acetoacetate → 3-methyl-1-phenylpyrazol-5-one → antipyrin (phenazone)
4. Benzaldehyde → benzoin → benzil → 5,5-diphenylhydantoin
5. Phenylhydrazine → acetophenone phenylhydrazone → 2-phenylindole
6. Chlorobenzene → 1-chloro-2,4-dinitrobenzene → 2,4-dinitrophenylhydrazine

Spectral Analysis

Interpretation of pre-recorded UV-Vis, IR, NMR, Mass, Raman spectrum and characterisation of one organic compound

St. Aloysius (Autonomous) College, Jabalpur**Department of Chemistry**

<i>Class</i>	<i>Course Type</i>	<i>Course Code</i>	<i>Course Title (Theory/Practical)</i>	<i>Marks</i>	
M.Sc. III SEM	Practical	Course MCH 306	Physical Chemistry	Max: 50	Min: 18

Maximum Marks: 50**Minimum Marks: 20****Conductometry**

- To determine the strength of unknown (given weak) acid conductometrically using standard alkali solution(strong).
- To determine the strength of unknown (given strong) acid conductometrically using standard alkali solution(weak).
- To determine the strength of acid conductometrically using standard alkali solution in a mixture of acids
- To determine the dissociation constant of weak electrolyte and to verify Ostwald's dilution law.
- To determine the equivalent conductance of strong electrolyte at the several concentration and hence verify Onsagar equation.
- To find the solubility and solubility product of sparingly soluble salt conductometrically.

pH metry

- To determine the strength of unknown (given weak) acid pHmetrically using standard alkali solution(strong).
- To determine the strength of unknown (given strong) acid pHmetrically using standard alkali solution(weak).
- To determine the strength of acid pHmetrically using standard alkali solution in a mixture of acids

Potentiometry

- To determine the strength of unknown (given weak) acid potentiometrically using standard alkali solution (strong).
- To determine the strength of unknown (given strong) acid potentiometrically using standard alkali solution (weak).
- To determine the strength of acid potentiometrically using standard alkali solution in a mixture of acids

Spectrophotometry

- To verify Lambert-Beer's law using a spectrophotometer.

Enzyme Kinetics

- To study the effect of temperature on invertase enzyme activity and determine its optimum pH
- To study of the effect of substrate concentration on enzyme activity.
- Effect of enzyme concentration on enzyme activity.

